Chloral 75-87-6 | DTXSID7024744

Model Performance

Model	Data	

Weighted KNN model

5-fold CV (75%)		Training (75°	Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.85	0.69	0.86	0.67	0.86	0.78	

Model Results

Predicted value: 1.18

Global applicability domain: Inside

Local applicability domain index: 4.75e-01

Confidence level: 6.69e-01

Nearest Neighbors from the Training Set

Image not found

Chloral

Measured: 0.99 Predicted: 1.18 Image not found

Bromochloromethane

Measured: 1.41 **Predicted:** 1.50

Image not found

Trichloroacetic acid

Measured: 1.33 Predicted: 1.41

Image not found

Trichloroethylene Measured: 2.42 Predicted: 2.29